

## APPENDIX 1

### Program for Baselineing, Normalizing, Interpolating Then Calculating Spectral Overlap Integrals

5 C This program has a non-standard DO WHILE loop

INTEGER NPTS, NMAX, ROWS, ITER

INTEGER EOF1, FLERR1, FLERR2

INTEGER EOF2, FLERR3, FLERR4

10 INTEGER EOF3, FLERR5, FLERR6

INTEGER FLERR7

INTEGER i,j

CHARACTER\*30 fname1, fname2, fname3, fname4

CHARACTER\*30 fname5, fname6, fname7

15 PARAMETER(NMAX=3500, LAMDA=601)

REAL x,xx1 (NMAX) ,yy1 (NMAX),INTERV1

REAL xx2 (NMAX) ,yy2 (NMAX), INTERV2

REAL xx3 (NMAX), yy3 (NMAX),INTERV3

20 REAL yil (NMAX), yi2 (NMAX), yi3 (NMAX), yc (NMAX)

REAL area

CHARACTER\*1 SUBSTR, INITAR, LIGHT, INTMED

FLERR1=0

25 FLERR2=0

FLERR3=0

FLERR4=0

FLERR5=0

FLERR6=0

30 FLERR7=0

EOF1=0

EOF2=0

EOF3=0

INTERV1=0

35 INTERV2=0

INTERV3=0

area=0

write(\*,\*) 'Do you wish to output intermediate files? (Y/N)'

40 read(\*, '(A)') INTMED

write(\*,\*) 'Do you wish to process a substrate file? (Y/N)'

read(\*, '(A)') SUBSTR

45 IF ((SUBSTR.EQ.'Y') .OR. (SUBSTR.EQ.'y')) THEN

10014350.10204

```

ITER=0
do 5 ITER=1, NMAX
    xx1 (ITER)=0
    yy1 (ITER)=0
    yi1 (ITER)=0
    5 continue

write(*,*) 'Enter the name of the input substrate file:'
read(*, ' (A)') fname1

open
(UNIT=11,FILE=fname1,STATUS='OLD',IOSTAT=FLERR1,E
RR=101)

ROWS=0

do while ((EOF1.EQ.0) .AND. (ROWS.LT.NMAX))
    ROWS=ROWS+1
    Read (11,*,IOSTAT=EOF1) xx1 (ROWS), yy1 (ROWS)
end do

close (UNIT=11)
NPTS=0

IF (EOF1.NE.0) THEN
    NPTS=ROWS-1
    write(*, '(I4,1X,A12)') NPTS, 'points read.'
ELSE
    NPTS=ROWS
    write(*, '(A28, I4, A12)') 'Too many data points! First',
+                               NMAX, 'points read...'
END IF

call baseln(yy1,NPTS)

IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN

    write(*,*) 'Enter the name of the output substrate file:'
    read(*, ' (A)') fname2
    open
    (UNIT=12,FILE=fname2,STATUS='NEW',IOSTAT=FLERR2,
ERR=102)

    write(*,*) 'Writing data...'

END IF

```

10011390-102201  
102201-08541001

```

x=0
i=0
j=0
5
do 12 i=1, LAMDA
    x= (i-1)+200
10    call locate(xx1,NPTS,x,j)
    if ((j.eq.0). OR. (j.eq.NPTS)) then
        INTERV1=0
    else
15        INTERV1= ((yyl(j+1)-yyl(j)) / (xx1(j+1) - xx1(j))) *
        (x-xx1(j))
        +          +yyl(j)
    end if
20    yi1 (i)=INTERV1
    IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
25        if ((j.eq.0) .OR. (j.eq.NPTS)) then
            GO TO 12
        else
            write(12,'(1x, f7.2,i6,3f12.2)')x,j,xx1(j),xx1(j+1),
+            INTERV1
30            endif
        END IF
35        12 continue
        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
            close (UNIT=12)
        END IF
40        ELSE
            ITER=0
            do 14 ITER=1, LAMDA
                yi1 (ITER) =1
45                14 continue
            ENDIF

```

10014300-102201  
102201-04241001

```

write(*,*) 'Do you wish to process an initiator file? (Y/N)'
read(*, '(A)') INITAR

5      IF ((INITAR.EQ.'Y') .OR. (INITAR.EQ.'y')) THEN

          ITER=0

          do 15 ITER=1,NMAX
10              xx2 (ITER) =0
                  yy2 (ITER) =0
                  yi2 (ITER) =0
15              continue

15      write(*,*) 'Enter the name of the initiator file:'
          read(*, '(A)') fname3

          open
          (UNIT=13,FILE=fname3,STATUS='OLD',IOSTAT=FLERR3,
20          ERR=103)

          ROWS=0

          do while ((EOF2.EQ.0) .AND. (ROWS.LT.NMAX))
25              ROWS=ROWS+1
                  read(13,*,IOSTAT=EOF2) xx2 (ROWS), yy2 (ROWS)
          end do

          close (UNIT=13)

30      NPTS=0

          IF (EOF2.NE.0) THEN
              NPTS=ROWS-1
35              write(*,1(14,1X,A12)) NPTS,'points read.'
          ELSE
              NPTS=ROWS
              write (*, '(A28,I4,A12)') 'Too many data points! First ',
+                  NMAX,' points read...'
40              END IF
                  call baseln (yy2,NPTS)

          IF ((INTMED.EQ.'Y').OR. (INTMED.EQ.'y')) THEN

45              write(*,*) 'Enter the name of the output initiator file: '
                  read(*, '(A)') fname4

```

10014390-102204  
102204-0824001

```

open
(UNIT=14,FILE=fname4,STATUS='NEW',IOSTAT=FLERR4,
ERR=104)

5       write(*,*) 'Writing data...'

      END IF
      x=0
      i=0
10     j=0

      do 22 i=1,LAMDA
          x=(i-1)+200

15         call locate (xx2,NPTS,x,j)
         if ((j.eq.0).OR. (j.eq.NPTS)) then
             INTERV2=0
             else
                 INTERV2= ((yy2(j+1)-yy2(j)) / (xx2(j+1) - xx2
20         (j))) * (x-xx2 (j))
                 + yy2 (j)
             end if
             yi2 (i)=INTERV2
             IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
25                 if ((j.eq.0) .OR. (j.eq.NPTS)) then
                     GO TO 22
                 else
                     write(14,'(1x,f7.2,i6,3f12.2)') x, j, xx2
30         (j),xx2 (j+1),
                     + INTERV2

                     endif
35         END IF

22         continue

40     IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
        close (UNIT=14)

      END IF
      ELSE
45         ITER=0

```



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```
        read(*,' (A)') fname6
        open
        (UNIT=16,FILE=fname6,STATUS='NEW',IOSTAT=FLERR6,
5         ERR=106)
```

```
        write(*,*) 'Writing data...'
```

```
    END IF
```

```
    x=0
```

10

```
    i=0
```

```
    j=0
```

```
    do 32 i=1,LAMDA
```

```
        x= (i-1)+200
```

15

```
        call locate (xx3,NPTS,x,j)
```

```
        if ((j.eq.0) .OR. (j.eq.NPTS)) then
```

```
            INTERV3=0
```

```
        else
```

20

```
            INTERV3= ((yy3(j+1) - yy3(j)) / (xx3(j+1) -
xx3(j))) * (x-xx3 (j))
```

```
            +
```

```
            +yy3 (j)
```

```
        end if
```

```
        yi3 (i) =INTERV3
```

```
        IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
```

25

```
            if ((j.eq.0).OR. (j.eq.NPTS)) then
```

```
                GO TO 32
```

```
            else
```

```
                write(16,'(1x,f7.2,i6,3f12.2)') x,j,xx3 (j),xx3 (j+1),
```

30

```
                +
```

```
                INTERV3
```

```
            endif
```

```
    END IF
```

35

```
    32          continue
```

```
    IF ((INTMED.EQ.'Y') .OR. (INTMED.EQ.'y')) THEN
```

```
        close (UNIT=16)
```

40

```
    END IF
```

```
    ELSE
```

```
    ITER=0
```

45

```
    do 34 ITER=1,LAMDA
```

```
        yi3 (ITER) -1
```

```
    34          continue
```

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ENDIF

ITER=0

5

DO 40 ITER=1,LAMDA

yc (ITER)=0

40 CONTINUE

10

DO 55 i=1,LAMDA

yc (i) =yi1 (i)\*yi2 (i)\*yi3 (i)

55 CONTINUE

write(\*,\*) 'Enter the filename for cumulative data:'

15

read (\*,'(A)') fname7

open

(UNIT=17,FILE=fname7,STATUS='NEW',IOSTAT=FLERR7,  
ERR=107)

write(\*,\*) 'Writing data...'

20

CALL integ (yc,LAMDA,area)

write(\*,'(1X,A26,A11,F12.6)') 'The area under the product',  
+'curve is:',area

25

write(17,'(1X,A26,A11,F12.6)') 'The area under the product',  
+'curve is:',area

DO 60 i=1,LAMDA

x= (i-1)+200

write(17,' (1X,F6.1,2F11.2,F11.4,E15.6)') x,yi1 (i),yi2

(i),

+ yi3 (i) ,yc (i)

60 CONTINUE

35

close (UNIT=17)

101 IF (FLERR1 .NE. 0) THEN

write(\*,\*) 'Unable to open substrate file!'

40

END IF

102 IF (FLERR2 .NE. 0) THEN

write(\*,\*) 'Unable to create substrate output file!'

END IF

45

103 IF (FLERR3 .NE. 0) THEN

write(\*,\*) 'Unable to open initiator file!'



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```

5      END IF

      104  IF (FLERR4 .NE. 0) THEN
          write(*,*) 'Unable to create initiator output file!'
      END IF

      105  IF (FLERR6 .NE. 0) THEN
          write(*,*) 'Unable to open light source file!'
      END IF

10     106  IF (FLERR6 .NE. 0) THEN
          write(*,*) 'Unable to create light source output file!'
      END IF

15     107  IF (FLERR7 .NE. 0) THEN
          write(*,*) 'Unable to create cumulative output file!'
      END IF

      write(*,*) 'Program exiting normally...'

20     END

      SUBROUTINE locate (xx,n,x,j)
      INTEGER j,n
      REAL x,xx (n)
      INTEGER j1,jm,ju
      J1=0
      ju=n+1
10         if (ju-j1.gt.1) then
            jm= (ju+j1) /2
            if ((xx (n).ge.xx (1)) .eqv. (x.ge.xx (jm))) then
                j1=j m
            else
                ju=jm
35         endif
        goto 10
      endif
      if (x.eq.xx (1))then
          j=1
40     else if (x.eq.xx(n))then
          j=n-1
      else
          j=j1
      endif
45     return END

      SUBROUTINE baseln (yy,N)

```

100  
90  
80  
70  
60  
50  
40  
30  
20  
10

```

INTEGER N, i
REAL yy (N), minno, temp

5      minno=yy (1)
      i=0
      temp=0

      DO 10 i=2,N
10         IF (yy (i) .LT. minno) THEN
            minno=yy (i)
        END IF
        10      CONTINUE

15      i=0

      DO 20 i=1,N
            temp=yy (i)-minno
            yy (i)=temp
20      CONTINUE

      END

SUBROUTINE norm (yy,N)

25      INTEGER N, i
      REAL yy (N),maxno,temp

      maxno=yy (1)
      i=0
      temp=0

      DO 5 i=2,N
            IF (yy(i).GT.maxno) THEN
35                maxno=yy (i)
            END IF
            5      CONTINUE

      i=0

40      DO 10, i=1,N
            temp=yy (i)/maxno
            yy (i)=temp
            10      CONTINUE

45      END

```



## APPENDIX 2

### Program to create uniformly spaced csv data from unevenly spaced tabular data

```
5      #include <stdio.h>
      #include <stdlib.h>
      #include <math.h>

10     #define NMAX 3501
      #define STRMAX 151
      #define FNMAX 81
      #define OUTPTS 801

15     void locate(float xx[], unsigned long n, float x, unsigned long *j);
      void norm(float xx[], unsigned long int n);
      void baseline(float xx[], unsigned long int n);

      int main()
20     {
      char fnamein(FNMAX), string[STRMAX], *str, ptr,
      fnameout[FNMAX], another;
      float xdata(NMAX), ydata[NMAX], xinter[OUTPTS+1],
      yinter[OUTPTS+1];
25     unsigned long int index, i, j;
      int choice;
      FILE *fpin, *fpout;

      another = 'Y';

30     do {
      for (i = 0; i <= NMAX-1; i++) {
      xdata [i] = 0;
      ydata [i] = 0;

35     };

      for (i = 0; i <= OUTPTS; i++) {
      xinter [i] = 0;
      yinter (i) = 0;

40     };

      printf("Enter name of the input file (80 chars max, no spaces): ");
      scanf("%s", fnamein);

45     printf("File name is %s\n",fnamein);

      fpin = fopen(fnamein,"r");

      if (fpin == NULL) {
```

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```
        printf("Cannot open %s\n",fnamein);
        exit(1);
    };

5      index = 1;

    while (1) {
        str_ptr = fgets(string,STRMAX-1,fpin);
        if(str_ptr == NULL)
10         break;
        if (index == NMAX)
            break;
        sscanf (string, "%f %f" , &xdata [index] , &ydata [index]);
        index++;
15    };

    fclose (fpin);

    if((index == NMAX) && (str_ptr != NULL)) {
        index--;
        printf("Too many data points! Using first %d points
only...\n",index);
    }
    else {
25         index--;
        printf("%d points read...\n",index);
    };

    printf("\nEnter option for data processing\n");
    printf("1: Normalize the data after interpolation\n");
    printf("2: Baseline the data after interpolation\n");
    printf("3: First interpolate, then baseline and finally ");
    printf("normalize the data\n");
    printf("4: Simply interpolate the data\n");
35    printf("5: Simply normalize the data\n");
    printf("6: Simply baseline the data\n");
    printf("or\n");
    printf("0: to exit the program without any data processing\n");
    printf("\nEnter option (0-6): ");
40    scanf("%d",&choice);

    if (choice == 0)
        exit(2);

45    printf("\nEnter name of the output file (80 chars max, no spaces): ");
    scanf("%s",fnameout);

    printf("File name is %s\n",fnameout);
```

```

fpout = fopen(fnameout,"w");

if (fpout == NULL) {
    printf("Cannot open %s\n",fnameout);
    exit(3);
};

for(i = 1; i <= OUTPTS; i++) {
    xinter[i] = 200+((float)i-1);
    locate(xdata,index,xinter[i],&j);
    if ((j == 0) || (j == index))
        yinter[i] = 0;
    else
        yinter [i] = (xinter [i] -xdata [j ]) * ((ydata (j+1] -ydata [j ]) /
            (xdata [j+1] -xdata [j ])) +ydata [j ] ;
};

if ((choice == 2) || (choice == 3)) {
    baseline(yinter,OUTPTS);
};

if (choice == 6) {
    baseline(ydata,index);
};

if ((choice == 1) || (choice == 3)) {
    norm(yinter,OUTPTS);
};

if (choice == 5) {
    norm(ydata,index);
};

if ((choice >= 1) && (choice <= 4)) {
    for (i = 1; i <= OUTPTS-1; i++) {
        fprintf(fpout,"%13.5E, ",yinter[i]);
    };
    fprintf(fpout,"%13.5E\n",yinter[OUTPTS]);
}
else
    if ((choice == 5) || (choice == 6)) {
        for (i = 1; i <= index-1; i++)
            fprintf(fpout,"%13.5E, ",ydata[i]);
        };
        fprintf(fpout,"%13.5E\n",ydata[index]);
    };

fclose(fpout);

```

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```

        printf("File %s written.\n\n",fnameout);
        printf("Process another file (Y/y/N/n)?: ");
        scanf("%ls",&another);
    } while (another == 'Y' || another == 'y');

    printf("Exiting...\n");
    return(0);
}

void locate(float xx[], unsigned long n, float x, unsigned long *j)
{
    unsigned long ju,jm,jl;
    int ascnd;

    jl=0;
    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (ju-jl > 1) {
        jm=(ju+jl) » 1;
        if (x >= xx[jm] == ascnd)
            jl=jm;
        else
            ju=jm;
    }
    if (x == xx[jl])
        *j=jl;
    else if (x == xx[ju])
        *j=ju;
    else
        *j=jl;
}

void norm(float xx[], unsigned long int n)
{
    unsigned long int i;
    float maxdata, temp;

    maxdata = xx[1];
    temp = 0;

    for(i = 2; i <= n; i++) {
        if(xx[i] > maxdata)
            maxdata = xx[i];
    };

    for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
    };
}

```

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}

void baseline(float xx[], unsigned long int n)

{

5

unsigned long int i;

float mindata, temp;

mindata = xx [ 1 ] ;

temp = 0;

10

for(i = 2; i <= n; i++) {

if(xx[i] < mindata)

mindata = xx [i] ;

};

15

for(i = 1; i <= n; i++) {

temp = xx(i) - mindata;

xx(i) = temp;

};

}



### APPENDIX 3

#### Program for Determining Strength of Wavelength Response in a Region

5

```
#include
<stdio.h>
#include
<stdlib.h>
#include
<math.h>

#define NMAX
3501
#define STRMAX
151
#define FNMAX
81
#define OUTPTS
801

void locate(float xx[], unsigned long n, float x,
unsigned long *j);
void norm(float xx[], unsigned long
int n);
void baseline(float xx[], unsigned
long int n);
void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
float *area);

int
main()
{
char fnamein[FNMAX], string[STRMAX], *str_ptr,
fnameout[FNMAX], another;
float xdata[NMAX], ydata[NMAX], xinter[OUTPTS+1],
yinter[OUTPTS+1];
float
totalarea,aA,aB,aC,aD,aE,aF,aG,aH,aI,aJ,a
K;
unsigned long int index, i,
j;
int choice;
FILE *fpin,
*fpout;
```

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```

another = 'Y';

printf("Contact Rajdeep S. Kalgutkar, SRC-CRC 7-3003, for
further info\n");

do {
    for (i = 0; i <= NMAX-1;
i++) {
        xdata[i]=0;
        ydata[i]=0;
    };

    for (i = 0; i <= OUTPTS;
i++) {
        xinter[i]=0;
        yinter[i]=0;
    };

    printf("\nEnter name of the input file (80 chars max, no
spaces): ");
    scanf("%s",fnamein);

    printf("File name is
%s\n",fnamein);

    fpin =
fopen(fnamein,"r");

    if (fpin ==
NULL) {
        printf("Cannot open %s.
Exiting...\n",fnamein);
        exit(1);
    };

    index = 1;

    while (1) {
        str_ptr = fgets(string,STRMAX-
1,fpin);
        if(str_ptr == NULL)
            break;
        if(index == NMAX)
            break;
        sscanf(string,"%f
%f",&xdata[index],&ydata[index]);

```

```

        index++;
    };

    fclose(fpin);

    if((index == NMAX) && (str_ptr != NULL)) {
        index--;
        printf("Too many data points! Using first %d points
only...\n",index);
    }
    else {
        index--;
        printf("%d points
read...\n",index);
    };

    printf("\nEnter option for data
processing\n");
    printf("1: Simply interpolate the
data\n");
    printf("2: Normalize the data after
interpolation\n");
    printf("3: Baseline the data after
interpolation\n");
    printf("4: First interpolate, then baseline and finally
");
    printf("normalize the
data\n");
    printf("or\n");
    printf("0: to exit the program without any data
processing\n");
    printf("\nEnter option (0-
4): ");
    scanf("%d",&choice);

    if (choice == 0)

exit(2);

    printf("\nEnter name of the output file (80 chars max, no
spaces): ");
    scanf("%s",fnameout);

    printf("File name is
%s\n",fnameout);

    fpout =

```

```

fopen(fnameout,"w");

if (fpout ==
NULL){
    printf("Cannot open %s.
Exiting...\n",fnameout);

exit(3);
};

for(i = 1; i <= OUTPTS;
i++) {
    xinter[i] = 200+((float)i-
1);
    locate(xdata,index,xinter[i],&j);
    if((j == 0) || (j ==
index))
        yinter[i] = 0;
    else
        yinter[i]=(xinter[i]-xdata[j])*((ydata[j+1]-
ydata[j])/
(xdata[j+1]-xdata[j]))+ydata[j];
};

if ((choice == 3) || (choice == 4)) {
baseline(yinter,OUTPTS);
};

if ((choice == 2) || (choice == 4)) {
norm(yinter,OUTPTS);
};

partinteg(yinter,51,OUTPTS,&totala
rea);

partinteg(yinter,51,101,&a
A);

partinteg(yinter,101,151,&
aB);

partinteg(yinter,151,201,&
aC);

```

```
partinteg(yinter,201,251,&
aD);
```

```
partinteg(yinter,251,301,&
aE);
```

```
partinteg(yinter,301,351,&
aF);
```

```
partinteg(yinter,351,401,&
aG);
```

```
partinteg(yinter,401,451,&
aH);
```

```
partinteg(yinter,451,501,&
aI);
```

```
partinteg(yinter,501,551,&
aJ);
```

```
partinteg(yinter,551,OUTPTS,&aK);
```

```
    fprintf(fpout,"The total area is:
%14.6E\n",totalarea);
    fprintf(fpout,"The area under region A is:
%6.2f%%\n",aA*100/totalarea);
    fprintf(fpout,"The area under region B is:
%6.2f%%\n",aB*100/totalarea);
    fprintf(fpout,"The area under region C is:
%6.2f%%\n",aC*100/totalarea);
    fprintf(fpout,"The area under region D is:
%6.2f%%\n",aD*100/totalarea);
    fprintf(fpout,"The area under region E is:
%6.2f%%\n",aE*100/totalarea);
    fprintf(fpout,"The area under region F is:
%6.2f%%\n",aF*100/totalarea);
    fprintf(fpout,"The area under region G is:
%6.2f%%\n",aG*100/totalarea);
    fprintf(fpout,"The area under region H is:
%6.2f%%\n",aH*100/totalarea);
    fprintf(fpout,"The area under region I is:
%6.2f%%\n",aI*100/totalarea);
    fprintf(fpout,"The area under region J is:
%6.2f%%\n",aJ*100/totalarea);
    fprintf(fpout,"The area under region K is:
%6.2f%%\n\n",aK*100/totalarea);
```

```

    for (i = 1; i <= OUTPTS-1; i++) {
        fprintf(fpout,"%13.5E, ",yinter[i]);
    };
    fprintf(fpout,"%13.5E\n",yinter[i]);

    fclose(fpout);

    printf("File %s
written.\n\n",fnameout);
    printf("Process another file
(Y/y/N/n)? : ");
    scanf("%1s",&another);
    } while (another == 'Y' || another
== 'y');

    printf("Exiting...\n
");

    return(0
);
}

void locate(float xx[], unsigned long n, float x,
unsigned long *j)
{
    unsigned long ju,jm,jl;
    int ascnd;

    jl=0;

    ju=n+1;
    ascnd=(xx[n] >= xx[1]);
    while (ju-jl > 1) {
        jm=(ju+jl) >> 1;
        if (x >= xx[jm] == ascnd)

    jl=jm;
    else

    ju=jm;
    }
    if (x == xx[1])
        *j=1;
    else if(x ==

```

```

xx[n])
*j=n-
1;
else
*j=j1;
}

```

```

void norm(float xx[], unsigned long
int n)

```

```

{
    unsigned long
    int i;
    float maxdata,
    temp;

```

```

    maxdata =
    xx[1];
    temp =
    0;

```

```

    for(i = 2; i <= n; i++) {
        if(xx[i] >
        maxdata)
            maxdata =
            xx[i];
    };

```

```

    for(i = 1; i <= n; i++) {
        temp = xx[i]/maxdata;
        xx[i] = temp;
    };
}

```

```

void baseline(float xx[], unsigned
long int n)

```

```

{
    unsigned long
    int i;
    float mindata,
    temp;

```

```

    mindata = xx[1];
    temp =
    0;

```

```

    for(i = 2; i <= n; i++) {
        if(xx[i] <

```

```

mindata)
    mindata =
xx[i];
};

for(i = 1; i <= n; i++) {
    temp = xx[i] - mindata;
    xx[i] = temp;
};
}

```

```

void partinteg(float xx[], unsigned long int x1, unsigned long int
x2,
float *area)
{
    unsigned long
int i;
float temp;

temp =
0;

for(i = x1; i <= x2 - 1; i++)
{
    temp = temp + (xx[i] + xx[i+1])/2;
};

*area = temp;
}

```

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#### APPENDIX 4

SRC Curing Resource dB 4 Query Select2

5 Sub Initialize

Dim ses ses As New NotesSession

Dim db\_db As NotesDatabase

Dim view view As NotesView

Dim note \_note1 As NotesDocument, note\_note2 As NotesDocument

10 Dim i cnt As Integer, i add As Integer

Set db\_db = ses ses.CurrentDatabase

Set note\_note1 = ses ses.DocumentContext

15 Redim Preserve arr WavelengthRegion(0) air WavelengthRegion(0) \_ ""

If note\_note1.Selection1(0) <> "" Or rwte\_note1.Selection2(0) <> "" Then

If note\_note1.Selection1(0) <> "" Then

Set view\_view = db\_db.GetView("By NoteID")

20 If note\_note1.Selection2(0) <> "" Then

Set note\_note2 = view\_view.GetDocumentByKey(Right("00000000" &  
note\_note1.Selection2(0), 8))

Else

25 Set note\_note2 = view\_view.GetDocumentByKey(Right("00000000" &  
note\_note1.Selection1(0), \$))

End If

If Not (note\_note2 Is Nothing) Then

30 If note\_note2.HasItem('WavelengthRegion') Then

i\_cnt = -1

Forall vals In note\_note2.WavelengthRegion

If vals <> "" Then

i\_cnt = i\_cnt + 1

35 Redim Preserve arr WavelengthRegion(i\_cnt)

arr\_WavelengthRegion(i cnt) = vals

End If

End Forall

40 End If

End If End If

If note\_note1.Type(0) = "S" Then

Set view-view = db\_db.GetView("Substrate")

45 Elseif note\_note1.Type(0) = "P" Then

Set view-view = db\_db.GetView("InitiatorSensitizer") Else

Set view-view = db\_db.GetView("LightSource") End If

```

' Set note note2 =view-view. GetFirstDocument

i_cnt = -1
5 Do While Not (note note2 Is Nothing)
  If note_note2.Name(0) <> "" Then
    L add = True
    If arr WavelengthRegion(0) <> "" Then
      Ladd = False
10 Forall vals1 In note_note2.WavelengthRegion
        Forall vals2 In arr_WavelengthRegion
          If vals1 = vals2 Then
            i_add = True
            Exit Forall
15         End If
        End Forall

        If Ladd Then
          Exit Forall
20      End If
    End Forall
    End If

    If L add Then
25         i cnt = i cnt + 1
        Redim Preserve arr_names(i cnt)
        arr names(i_cnt) = note_note2.Name(0)
    End If
    End It
30
    Set note note2 = view-view. GetNextDocument(note_note2)
  Loop

  note _note1.Names = arr_names
35 End Sub

SRC Curing Resource dB 4 Query Select2 Save Agent

Sub Initialize
40 Dim ses sesAs New NotesSession
  Dim db_db As NotesDatabase
  Dim view view As NotesView
  Dim note_note1 As NotesDocument, note_note2As NotesDocument

45 Set db_db = ses ses.CurrentDatabase
  Set note note) = ses ses.DocumentContext

```

```
Select Case note_notel.Type(0)
Case "S"
Set view view = db_db.GetView("(Substrate)")
```

5 Set note\_note2=view view.GetDocumentByKey(note\_notel.Substrate(0))

```
Case "P"
Set view-view db-db.GetView("(InitiatorSensitizer)")
```

10 Set note note2 -view view.GetDocumentByKey(note notel.PhotolInitiator(0))

```
Case "L"
Set view-view =db db.GetView("(LightSource)")
```

15 Set note\_note2 = view\_view.GetDocumentByKey(note\_notel.LightSource(0))

End Select

```
If note_notel.MexWction(0) = "Add" Then
```

20 If note\_notel.Selection1 (0) <> "" Then

```
Print "[!" + note notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_notel.Selection1 (0) & "&" & note_note2.Noteld & ")"
```

Else

25 Print "[!" + note notel.dbname(0) + "/QuerySelection1?OpenForm&" &  
note\_note2.Noteld & "]"

```
End If Elseif note notel.NextAction(0) = "Separate" Then
```

```
If note_notel.Selection1(0) <> "" Then
```

```
Print "[/" + note notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_notel.Selection1(0) & "&" & note note2.Noteld & ")"
```

30 Else

```
Print "[/" + note notel.dbname(0) + "/QuerySelection1?OpenForm&" &
note_note2.Noteld & ")"
```

End If

```
Elseif note_notel.NextAction(0) = "Separate" Then
```

35 If note\_notel.Selection2(0) <> "" Then

```
Print "[/" + note notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &
note_notel.Selection (0) & "&" & note note).Selection2(0) & _
"&" & note_note2.Noteld & "]"
```

```
Elseif note notel.Selection1(0) <> "" Then
```

40 Print- "[ + note notel.dbname(0) + "/QuerySelectionResults?OpenForm&" &  
note\_notel.Selection1 (0) & "&" & note note2.Noteld & ")"

Else

```
Print "[/" + note_notel.dbname(0) + "lQuerySelectionResults?OpenForm&" &
note_noteMoteld & "]"
```

45 End If

Else

```
If note notel.Selection2(0) <> "" Then
```

Print “[/” + note\_note1.dbname(0) + “/QuerySelectionOverlayResults?OpenForm&” &  
note\_note1.Selection1(0) & “&” & note\_note1.Selection2(0) &  
“&” & note\_note2.NoteId & “)”

Elseif note\_note1.Selection1(0) <> “” Then

5 Print “[/” + note\_note1.dbname(0) + “/QuerySelectionOverlayResults?OpenForm&”  
& note\_note1.Selection1(0) & “&” & note\_note2.NoteId & “)”

Else

Print “[/” + note\_note1.dbname(0) + “/QuerySelectionOverlayResults?OpenForm&”  
& note\_note2.NoteId & “)”

10 End If

End If

End Sub

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# SRC Curing Resource dB 4 Query Overlay Open Agent

## Sub Initialize

```
5      pim ses_ses As New NotesSession
      Dim db db As NotesDatabase
      Dim view-view As NotesView
      Dim note notel As NotesDocument. note_note2As NotesDocument
      Dim i_cntAs Integer, i addAs Integer

10     Set db db = ses ses.CurrentDatabase
     Set note notel =ses ses.DocumentContext

     S et view-view = db_db. G etView("By N otel D ")

15     If note notel.Selection1(0) <> "" Then
     S et note-note2 = view-view. G etD ocumentByKey(R ight("00000000" + note_notel.
     S election"! (0). 8))

20     If Not (note _note2 Is Nothing) Then
         note _notel.data1 = note _note2.EmissData
         note notel.maxfreq1 = note _note2.MaxFreq
     End If End If

25     If note _notel.Selection2(0) <> "" Then
     Set note-note2 = view view.GetDocumentByKey(Right("00000000" +
     note _notel.Selection2(0), 8))

30     If Not (note note2 Is Nothing) Then
         note notel.data2=note _note2.EmissData
         note _notel.maxfreq2 = note _note2.MaxFreq
     End If End If

35     If note notel.Selection3(0) <> "" Then
     Set note-note2 = view _view.GetDocumentByKey(Right("00000000" +
     note _notel.Selection3(0), 8))

40     If Not (note _note2Is Nothing) Then
         note notel.data3 = note note2.EmissData
         note _notel.maxfreq3=note note2.MaxFreq
     End If End If End Sub
```

## APPENDIX 5

```
import java.awt.*; import java.awt.event.*; import java.applet.*;
```

```
5 public class SRC Charts extends Applet { int gi count;
```

```
double GetHMax(String str_in) { String str_current; double dbl hmax;
```

```
str_current = ""; dblhmax = 0; for Tint i cnt = 0; i_cnt < str_in.length(); i cnt++) {
```

```
10 if(str in. region Match es(i cnt, "", 0, 2))
```

```
if(Double.valueOf(str current).doubleValue() > dbl_hmax)
```

```
dbl hmax = Double.valueOf(str current).doubleValue();
```

```
str current = "" ;
```

```
i_cnt++;
```

```
15 gi count++; ) else {
```

```
str current = str current.concat(str in.substring(i cnt, i cnt + 1));
```

```
)
```

```
if(str_current.length() > 0) {
```

```
20 if(Double.valueOf(str_current).doubleValue() > dbl_hmax)
```

```
dbl hmax = Double.valueOf(str_current).doubleValue(); gi count++; ) return dbl hmax;
```

```
int StringToInt(String str_in, double dbl hmax) { double dbl_pos;
```

```
25 dbl_pos = getSize().height - (25 + (Double.valueOf(str_in).doubleValue() *  
((getSize().height - 50) / dbl hmax))); return (int)dbl-pos; )
```

```
void drawChartLine(Graphics g, String str_in, String str_type, double dbl_maxfreq) {  
30 double dbl_x, dbl_inc, dbl_hmax; String str last, str next;
```

```
str last str_next = "" ; dbl x = 25; gi count = 0;
```

```
dbl_hmax = GetHMax(str_in); if(str type. equals IgnoreCase("S")) dbl hmax = 100;
```

```
35
```

```
dbl inc = (((double)getSize().width - 50) / gi count) * ((dbl maxfreq - 200) / 800));
```

```

for (int i cnt = 0; i_cnt < str_in.length(); ) “, “, i c{
    nt++)if(str_in.regionMatches(i cnt, 0,
5    2))if(str_last.length(> 0)    {
    {
    g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl inc),
    StringToInt(str_next, dbl hmax));
    dbl x = dbl x + dbl inc;

10    str last = str_next; str next = “”; i cnt++;

    else { str next = str next.concat(str in.substring(i cnt, i cnt + 1));

    )
15    if(str_next.length() > 0)
    g.drawLine((int)dbl x, StringToInt(str_last, dbl hmax), (int)(dbl x + dbl-inc),
    StringToInt(strnext, dbl_hmax)); )

    public void paint(Graphics g) { double dbl x, dbl-y;

20    g.setColor(Color.black); g.drawLine(0, 0, getSize().width, 0); g.drawLine(25,
    getSize().height - 25, getSize().width - 25, getSize().height - 25); g.drawLine(25, 25,
    25, getSize().height - 25);

25    for(int i cnt = 0; i_cnt < 9; i cnt++) {
    dbl_x = 25 + (((double)i cnt * (((double)getSize().width - 50) / 8));
    g.drawLine((int)dbl x, getSize().height - 25, (int)dbl x, getSize().height - 20);
    g.drawString(String.valueOf((i cnt * 100) + 200), (int)dbl x - 8, getSize().height - 5); )

30    for(int i cnt = 0; i_cnt < 11; i_cnt++) {
    dbl-y = 25 + (((double)i cnt * (((double)getSize().height - 50) / 10));
    g.drawLine(20, (int)dbl-y, 25, (int)dbl-y);
    g.drawString(String.valueOf(100 - (i cnt * 10)), 1, (int)dbl-y + 5); )

35    g.drawString(“Data Overlay”, (getSize().width / 2) - 30, 12);

    g.setColor(Color.red); drawChartLine(g, getParameter(“Data 1 “), getParameter(“Type
    1 “), Double.valueOf(getParameter(“Max Freq 1 “)).doubleValue());
    g.setColor(Color.blue); drawChartLine(g, getParameter(“Data 2”),
40    getParameter(“Type 2”), Double.valueOf(getParameter(“Max Freq
    2”)).doubleValue()); g.setColor(Color.green); drawChartLine(g, getParameter(“Data
    3”), getParameter(“Type 3”), Double.valueOf(getParameter(“Max Freq
    3”)).doubleValue()); )

```